Linear Harmonic Oscillator

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We are to ~~solve the~~ obtain the solution of 1D schrodinger equation corresponding to the linear harmonic oscillator. Then we ~~fi~~ will find the time evolution of coherent states of the oscillator and represents the quantum mechanical analogue to the classical operator.

The One dimensional time dependent Schrodinger equation is given by

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi(x,t) \longrightarrow (1)$$

$$\text{where } H = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x) \longrightarrow (11)$$

The quantum problem is to solve the Schrodinger equation for the potential

$V = \frac{1}{2}m\omega^2x^2$ where in the conventional potential of harmonic oscillator ~~V=k~~ $V = \frac{1}{2}kx^2$, The force constant k is replaced by the classical frequency ω, using the relation $\omega = \sqrt{\frac{k}{m}}$; $\Rightarrow K = \omega^2 m$

Now we are ready to solve the Time independent Schrodinger Eqn

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$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi \longrightarrow \text{(III)}$$

To solve the equation (iii) we introduce a dimensionless variable $\xi=\sqrt{\frac{m\omega}{\hbar}}\,x \longrightarrow$ (IV)

$$\therefore \frac{d\xi}{dx}=\sqrt{\frac{m\omega}{\hbar}}$$

Now $\frac{d\psi}{dx}=\frac{d\psi}{d\xi}\frac{d\xi}{dx}=\frac{d\psi}{d\xi}\sqrt{\frac{m\omega}{\hbar}}$

$$\frac{d^2\psi}{dx^2}=\frac{d}{dx}\left(\frac{d\psi}{dx}\right)=\frac{d}{d\xi}\left(\frac{d\psi}{d\xi}\frac{d\xi}{dx}\right)\frac{d\xi}{dx}$$

$$=\frac{d^2\psi}{d\xi^2}\left(\frac{m\omega}{\hbar}\right), \quad \xi^2=\frac{m\omega x^2}{\hbar}$$

Now changing the variable equation (iii) takes the form.

$$-\frac{\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)\frac{d^2\psi}{d\xi^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi$$

Multiplying both sides by $2/\hbar\omega$ of the above equation we have

$$-\frac{d^2\psi}{d\xi^2}+\frac{m\omega x^2}{\hbar}\psi=\frac{2E}{\hbar\omega}\psi$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2}-\xi^2\psi=-K\psi \qquad \text{where } \frac{2E}{\hbar\omega}=K \longrightarrow \text{(V)}$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2}=(\xi^2-K)\psi \longrightarrow \text{(VI)}$$

Solving equation (VI) we will obtain the allowed

values of k.

We consider the point that for large values of ξ, ξ^2 dominates over k and equation (vi) reduces to

$$\frac{d^2\psi}{d\xi^2} = \xi^2\psi \longrightarrow \text{(vii)}$$

The general solution of equation (vii) is of the form

$\psi(\xi) = A e^{-\xi^2/2} + B e^{+\xi^2/2}$, the second part of the solution is not normalizable because it blows up as $|\xi| \to \infty$

The acceptable solution $\psi(\xi) = \text{Const}\ e^{-\xi^2/2}$

or $\psi(\xi) = h(\xi)\ e^{-\xi^2/2} \longrightarrow \text{(viii)}$

Differentiating equ^n (viii) twice w.r.t ξ.

$$\frac{d^2h(\xi)}{d\xi^2} - 2\xi\frac{dh(\xi)}{d\xi} + (k-1)h(\xi) = 0 \longrightarrow \text{(ix)}$$

Rough

$$\frac{d\psi(\xi)}{d\xi} = \left[\frac{dh(\xi)}{d\xi} - \xi h(\xi)\right] e^{-\xi^2/2}$$

$$\frac{d^2\psi(\xi)}{d\xi^2} = \left[\frac{d^2h(\xi)}{d\xi^2} - 2\xi\frac{dh(\xi)}{d\xi} + (\xi^2-1)h(\xi)\right] e^{-\xi^2/2}$$

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It is seen that ~~the~~ when $\xi \to \pm\infty$, the solution of equation (ix) diverge like e^{ξ^2}

unless K has one of the values $K = (2n+1)$
(for $n = 0, 1, 2 \cdots$)

$\therefore$ The admissible values of $\psi(\xi)$ exists only for some special values of K, corresponding to

the energy value $E_n = (n + \frac{1}{2})\hbar\omega$ —— (x)

These are the expression of energy ~~so~~ eigenvalues of the simple harmonic oscillator.

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Let $h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$

$$\frac{dh(\xi)}{d\xi} = \sum_j j a_j \xi^{j-1}$$

$$\frac{d^2 h(\xi)}{d\xi^2} = \sum_j j(j-1) a_j \xi^{j-2}$$ (XI)

Using (XI) in equation (IX)

$$\sum j(j-1) a_j \xi^{j-2} - 2\sum j a_j \xi^j + (K-1)\sum a_j \xi^j = 0$$

$$\Rightarrow \sum j(j-1) a_j \xi^{j-2} = (2j - K + 1)\sum a_j \xi^j$$

Equating the co-eff of ξ^j from both sides of the above equation.

$$(j+2)(j+1)a_{j+2} = (2j+1-K)\, a_j$$

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)}\, a_j \longrightarrow (XII)$$

This recursion formula is entirely equivalent to the schrodinger equation. Starting with a_0, it generates all the even number co-efficients.

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The equation is (XII) determines $h(\xi)$ in terms of arbitrary constants a_0 and a_1.

Which is just what would we expect for a 2nd order differential equation.

Not all the solutions so obtained are ~~not~~ normalizable.
For very large j, the recursion formula becomes

$$a_{j+2} \simeq \frac{2}{j} a_j \longrightarrow \text{(XIII)}$$

with the approximate solution $a_j = \frac{C}{(j/2)!}$

For some const C, and this yields at large ξ,

where the higher power dominate.

$$h(\xi) = C \sum \frac{1}{(j/2)!} \xi^{j} = C \sum \frac{1}{j!} \xi^{2j} \simeq C e^{\xi^2}$$

Now if $h(\xi)$ goes like $\exp(\xi^2)$, then ψ goes like $\xi^2/2$.

For normalizable solutions, the power series must terminate. There must occur some higher value of j for which the recursion formula splits out. Let the highest value of j is n

$\therefore a_{n+2} = 0$

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This will ~~truncate~~ terminate either the h even or hodd series.

If n is even $a_1 = 0$,
& if n is odd $a_0 = 0$.

For a physically acceptable solution it requires.

$$a_{j+2} = \frac{2j+1-K}{(j+1)(j+2)} = 0 \Rightarrow 2j+1-K = 0$$

↑ (XIV)   for $j = n$
$K = 2n+1$

$$K = \frac{2E}{\hbar\omega} = 2n+1$$

$$\Rightarrow E = \left(n+\tfrac{1}{2}\right)\hbar\omega \qquad n = 0, 1 \ldots$$

The equation $H\psi = E\psi$ has solutions of course for any value of E, there are two linear independent solution for every E.

For allowed values of K, the recursion formula (XIV) reads.

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j \quad \text{Putting } K = 2n+1$$

——— (XIX)

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For $n=0$,

There is Only one term in the series and a_1 must ~~must be 0 to~~ vanish the hood.

for $j=0$, equ^n (X1X) becomes $h_0(\xi)=a_0$

$$\boxed{\psi_0(\xi)=C_0\, e^{-\xi^2/2}}$$

For $n=1$ we ~~...~~ take $a_0=0$, $j=1$

$a_3=0$

$h_1(\xi)=a_1\xi$

$$\therefore\ \boxed{\psi_1=a_1\xi\, e^{-\xi^2/2}}$$

for $n=2$, $j=0$

$a_2=-2a_0$

for $n=2$, $j=2$

$a_1=0$

$h_2(\xi)=a_0(1-2\xi^2)$

$\psi_2(\xi)=a_0(1-2\xi^2)\,e^{-\xi^2/2}$

For an even n, $h(\xi)$ is a polynomial of degree n, involving even powers Only.

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For an odd n, $h_n(\xi)$ contains odd powers only.

All the terms are called Hermite polynomials $H_n\xi$

— x

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Topic → Quantum Mechanics of Simple harmonic oscillator.
energy level, energy eigenfunction. using Frobenous method. ground state, zero point energy.

☐ Application

→ To understand and study the vibrational spectra of molecules,

☐ In the study of quantum theory of radiation.